

## High Oxidation State Metal Complexes: New Reactions, Applications, and Tools for Catalyst Development

Aaron Odom

Department of Chemistry  
Michigan State University

In our laboratory, we have developed new methods for catalyst parameterization that allow rational catalyst development for high valent systems. The method allows us to parameterize the donor ability of many common ligands towards metals in a high oxidation state. One chart showing a few of the ligands we have examined is above. Ligands with small Ligand Donor Parameters (LDP) are better donors, while those with larger values are poor donors. Multivariate analysis can be used with LDP and a steric parameter to model a series of catalysts. The model can then be used to predict the rates of catalysts that have not been prepared. In addition, interesting mechanistic information can be gleaned from these types of studies that is not available from more traditional mechanistic methods. Recently, we published a simple method for high oxidation state ligand parameterization, and we are following up on applying the system to optimization of several different catalytic systems, including our own titanium-catalyzed multicomponent coupling chemistry.

